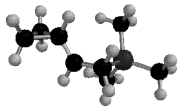
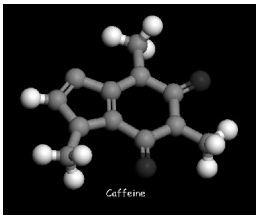
Organic Chemistry

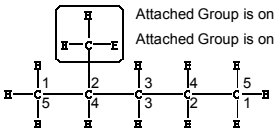


Nomenclature:
Alkanes



Step 2. Number the parent chain.

- Number the parent chain so that the substituent (attached) groups are on the lowest numbers



Organic Compound Classification

- Have hydrocarbon chains (carbon & hydrogen)
- Saturated – no double bonds
- Unsaturated: has double or triple bonds

Type	Kinds of Bonds	Suffix
Alkane	Single only	-ane
Alkene	Single and double	-ene
Alkyne	Single & triple	-yne
Substituent Groups	Single (but not part of the longest chain)	-yl

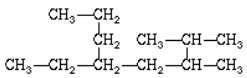
Prefixes for # of Carbons

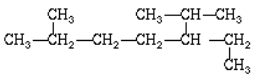
1	Meth	6	Hex
2	Eth	7	Hept
3	Prop	8	Oct
4	But	9	Non
5	Pent	10	Dec

- Regardless of type (alkane, alkene, alkyne or substituent group)

Step 1. Find the "Parent Chain"

- Where is the longest continuous chain of carbons that does not double back?





Step 3. Name the attached groups.

- Carbon (alkyl) groups (Carbon & Hydrogen Only)
  - Methyl CH_3 -
  - Ethyl CH_3CH_2-
  - Propyl $CH_3CH_2CH_2$
- Specific Functional Groups
  - Halogens (F, Cl, Br, I)
  - Amines (NH_2)
  - Nitriles ($C \equiv N$)

Functional Groups & Priority

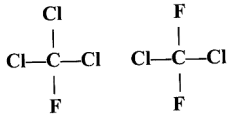
Priority	Type	Molecular	Formula	Prefix	Suffix
1	Ester	C-COO-C	C-C(=O)-O-C	---	-oanate
2	Carboxylic Acid	C-COOH	C-C(=O)-O-H	Carboxyl-	-oic acid
3	Amide	C-CONH$_2$	C-C(=O)-NH$_2$	Carbamide	-amide
4	Nitrile	C-C≡N	C-C≡N	Cyano-	-nitrile
5	Aldehyde	C-CHO	C-C(=O)-H	Oxo-	-al
6	Ketone	C-COO-C	C-C(=O)-O-C	Oxo-	-one
7	Alcohol	C-C-OH	C-C-O-H	Hydroxyl-	-ol
8	Amine	C-C-NH$_2$	C-C-NH$_2$	Amino	-amine
9	Ether	C-CO-C	C-C-O-C	---	Ether
10	Halogen	R-X	R-X	Halo-	---
11	Alkyl	C-C	C-C-C	Alkyl	---

Step 6. Give the name of the longest chain with the appropriate ending

- If no functional group is listed shown, use the ending –ane, -ene, -yne.
- If there is a functional group, use the ending listed
  - If more than 1 functional group use the one with a higher priority.

Step 4. Alphabetize & combine like groups.

- The prefixes di, tri, tetra instead of saying the same group multiple times
- Prefixes are not considered when alphabetizing (Example: dimethyl = use the m from methyl for alphabetizing

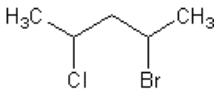


Freon-11
1,1,1-trichloro-1-fluoromethane

Freon-12
1,1-dichloro-1,1-difluoromethane

Other Order of Priority

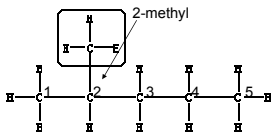
- IN A TIE between SIMILAR GROUPS, the group lower ALPHABETICALLY gets the lower number



4-bromo-2-chloropentane or
2-bromo-4-chloropentane ?

Step 5. Tell where the group is attached to the parent chain.

- Use the numbers of the parent chain for location of the attached groups
- List substituents alphabetically. Use commas to separate numbers and dashes between word and numbers

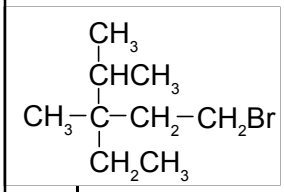


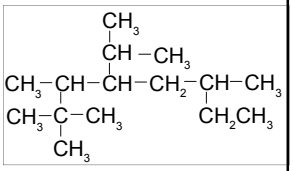
Draw Some Simple Alkanes

- 2-methylpentane
- 3-ethylhexane
- 2,2-dimethylbutane
- 2,3-dimethylbutane

Alkanes

Example: Name the following compounds:





Isomers

- Straight chain alkanes: An alkane that has all its carbons connected in a row.
- Branched chain alkanes: An alkane that has a branching connection of carbons.
- Isomers: Compounds with same molecular formula but different structures.

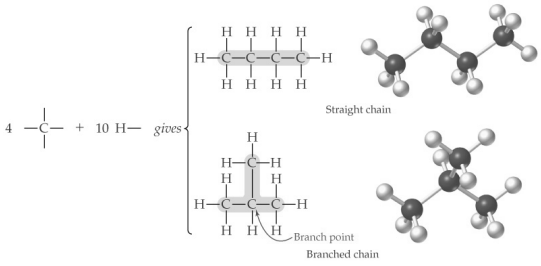
Alkanes

Example: Write the structure for the following compounds:

3,3-dimethylpentane

2-methyl-4-sec-butyloctane

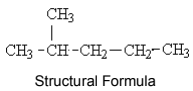
1,2-dichloro-3-methylheptane



- The Carbons in butane (C_4H_{10}) can be arranged in two ways
  - four carbons in a row (linear alkane) or a
  - branching (branched alkane).

Structural Formulas

- "Lazy" way to write the Hydrogens
- Instead of drawing the bonds, just state how many hydrogens are attached
- NOTE: The bonds are between CARBONS in a parent chain, and not hydrogens!


Structural Formula

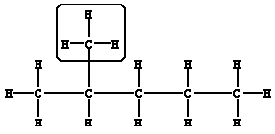
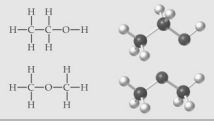

Lewis Structure

TABLE 12.3 Some Properties of Ethyl Alcohol and Dimethyl Ether

Name and Molecular Formula	Structure	Boiling Point	Melting Point	Physiological Activity
Ethyl alcohol C_2H_6O		78.5°C	−117.3°C	Central-nervous-system depressant
Dimethyl ether C_2H_6O		−23°C	−138.5°C	Nontoxic; anesthetic at high concentration

- Different isomers are completely different compounds.
  - Structures
  - physical properties
    - melting point
    - boiling point
  - physiological properties.

TABLE 12.5 Some Common Alkyl Groups*

CH_3- Methyl	CH_3CH_2- Ethyl	$CH_3CH_2CH_2-$ *n*-propyl	$CH_3CH(CH_3)-$ Isopropyl
$CH_3CH_2CH_2CH_2-$ *n*-Butyl	$CH_3CH(CH_3)CH_2CH_3$ *sec*-Butyl	$CH_3CH(CH_3)CH_2-$ Isobutyl	$CH_3C(CH_3)_2CH_3$ *tert*-Butyl

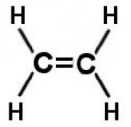
*The red bond shows the connection to the rest of the molecule.

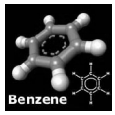
- Other "special naming issues"
  - n: Normal (straight chain)
  - iso: In the middle (only with odd numbered chains)
  - sec: 2 other carbons attached
  - tert: 3 other carbons attached

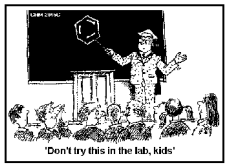
Naming Alkenes and Alkynes

- The longest chain must **contain** the **double or triple bond**,
- Name the parent compound by adding the suffix **–ene or –yne** to the name of the main chain if there is no functional group.

Special Naming Considerations Alkenes, Alkynes, and Aromatic Compounds



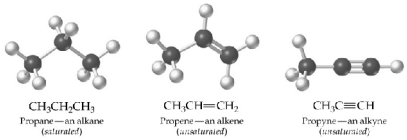




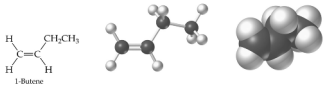
- **Step 2:** Number the carbon atoms in the parent chain, beginning at the end nearest to the double or triple bond. If the multiple bond is an equal distance from both ends, begin numbering at the end nearer the first branch point. The number indicates which carbon the multiple bond FOLLOWS. (i.e. between 2 and 3 is 2-)
- **Step 3:** Assign numbers and names to the branching substituents, and list the substituents alphabetically. Use commas to separate numbers, and hyphens to separate words from numbers.

Alkenes and Alkynes

- Unsaturated
  - contain carbon-carbon double and triple bond to which more hydrogen atoms can be added.
- Alkenes: carbon-carbon double bonds
- Alkynes: carbon-carbon triple bonds.



- **Step 4.** Indicate the position of the multiple-bond carbon. If more than one multiple bond is present, identify the position of each multiple bond and use the appropriate ending diene, triene, tetraene, and so forth.
- **Step 5.** Assemble the name.



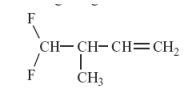
Naming Alkenes and Alkynes

When the carbon chain has 4 or more C atoms, number the chain to give the lowest number to the double or triple bond.

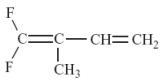
1 2 3 4

$CH_2{=}CHCH_2CH_3$	1-butene	but-1-ene
$CH_3CH{=}CHCH_3$	2-butene	but-2-ene
$CH_3C{\equiv}CCH_3$	2-butyne	but-2-yne

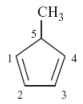
Multiple Double/Triple Bonds



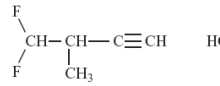
4,4-difluoro-3-methylbut-1-ene



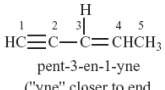
1,1-difluoro-2-methyl-buta-1,3-diene



5-methylcyclopenta-1,3-diene

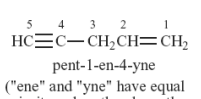


4,4-difluoro-3-methylbut-1-yne



pent-3-en-1-yne

("yne" closer to end of chain)



pent-1-en-4-yne

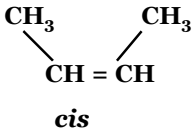
("ene" and "yne" have equal priority unless they have the same position number, when "ene" takes the lower number)

Assigning Priority

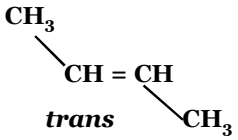
- In a molecule with both a double and a triple bond, whichever is closer to the end of the chain determines the direction of numbering.
- In the case where each would have the same position number, the double bond takes the lower number.
- In the name, "ene" comes before "yne" because of alphabetization.

Cis and Trans Isomers

- **Double bond is fixed**
- **Cis/trans Isomers are possible**



cis



trans

Learning Check

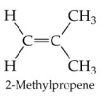
Write the name for each of the following unsaturated compounds:

A. $CH_3CH_2C{\equiv}CCH_3$

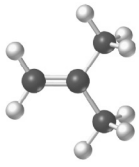
B. $CH_3C(CH_3){=}CHCH_3$

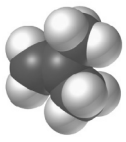
Cis-trans isomerism

- occurs in an alkenes only
- not possible if one of the double bonded carbons is attached to two identical groups.

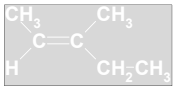


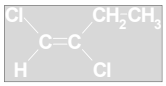
2-Methylpropene





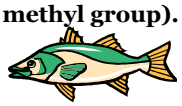
Name These





Omega-3 Fatty Acids

- **Fatty acids in the fish oils are mostly the omega-3 type (first double bond occurs at the third carbon counting from the methyl group).**
- **linolenic acid 18 carbon atoms**



$CH_3CH_2CH=CHCH_2CH=CHCH_2CH=CH(CH_2)_7COOH$

↑

Unsaturated Fatty Acids

- **Fatty acids in vegetable oils are omega-6 acids (the first double bond occurs at carbon 6 counting from the methyl group)**
- **A common omega-6 acid is linoleic acid**

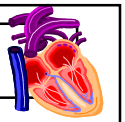
$CH_3CH_2CH_2CH_2CH_2CH=CHCH_2CH=CH(CH_2)_7COOH$

↑

6

linoleic acid, a fatty acid

Atherosclerosis



- **Plaques of cholesterol adhere to the walls of the blood vessels & blood pressure rises as blood squeezes through smaller blood vessels**
- **Blood clots may form**
- **Omega-3 fatty acids decrease the "sticking" of blood platelets (fewer blood clots) & can increase bleeding time**

Trans Fats

- **In vegetable oils, the unsaturated fats usually contain *cis* double bonds.**
- **During hydrogenation, some *cis* double bonds are converted to *trans* double bonds (more stable) causing a change in the fatty acid structure**

Polymers

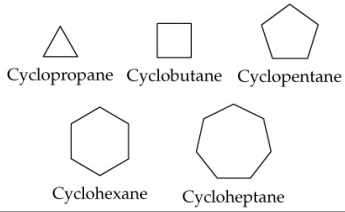
- Large molecules formed by repetitive bonding of samller molecules called monomers
  - Cellulose & Starch are built from simple sugars
  - Proteins are built from amino acids
  - DNA is built from nucleic acids
  - Fats are built from 3 fatty acids and a glycerine

TABLE 13.1 **Some Alkene Polymers and Their Uses**

Monomer Name	Monomer Structure	Polymer Name	Uses
Ethylene	$H_2C{=}CH_2$	Polyethylene	Packaging, bottles
Propylene	$H_2C{=}CH{-}CH_3$	Polypropylene	Bottles, rope, pails, medical tubing
Vinyl chloride	$H_2C{=}CH{-}Cl$	Poly(vinyl chloride)	Insulation, plastic pipe
Styrene	$H_2C{=}CH{-}C_6H_5$	Polystyrene	Foams and molded plastics
Styrene and butadiene	$H_2C{=}CH{-}C_6H_5$ and $H_2C{=}CHCH{=}CH_2$	Styrene-butadiene rubber (SBR)	Synthetic rubber for tires
Acrylonitrile	$H_2C{=}CH{-}C{\equiv}N$	Orlon, Acrilan	Fibers, outdoor carpeting
Methyl methacrylate	$H_2C{=}C(CH_3)COCH_3$	Plexiglas, Lucite	Windows, contact lenses, fiber optics
Tetrafluoroethylene	$F_2C{=}CF_2$	Teflon	Nonstick coatings, bearings, replacement heart valves and blood vessels

Drawing and Naming Cycloalkanes

Cycloalkanes are represented by polygons. A triangle represents cyclopropane, a square represents cyclobutane, a pentagon represents cyclopentane, and so on.



Nomenclature: Cyclic Alkanes

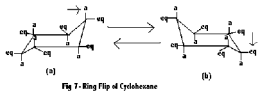
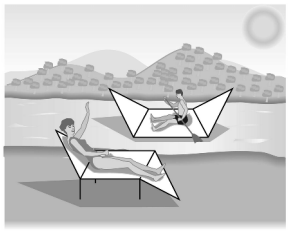
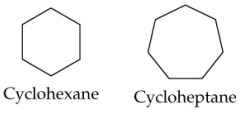
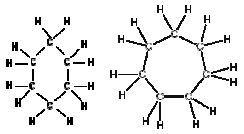


Fig 7- Ring Flip of Cyclohexane



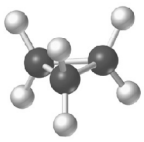
•***Line structure***: A shorthand way of drawing structures in which atoms aren't shown; instead a carbon atom is understood to be at each corner and hydrogens are "understood".

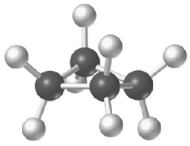


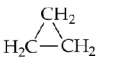


Cycloalkanes

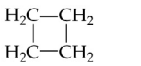
Cycloalkanes: An alkane that contains a ring of carbon atoms. Ring sizes from 3 carbons to 30 or higher are known.







Cyclopropane
(mp −128°C, bp −33°C)



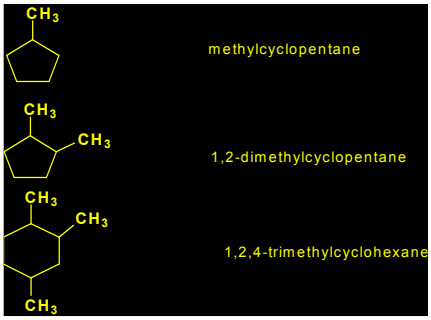
Cyclobutane
(mp −50°C, bp −12°C)

Additional Rules for Naming Cyclics

•**Step 1**: Use the prefix cyclo- with the parent chain.

•**Step 2**: Number the substituents starting at the group that has alphabetical priority, and proceed around the ring in the direction that gives the second substituent the lower possible number.

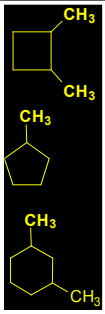
Cycloalkanes with Side Groups



Aromatic Compounds and the Structure of Benzene

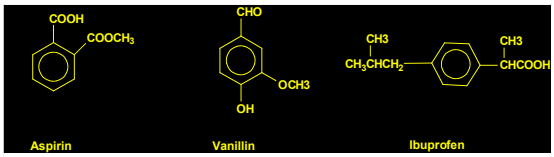
- In the early days the word *aromatics* was used to described many fragrant molecules isolated from natural sources. Today the term *aromatic* is used to describe benzene like molecules.
- It has alternating three carbon-carbon double and three single bonds.

Learning Check



Aromatic Compounds in Nature and Health

Many aromatic compounds are common in nature and in medicine.

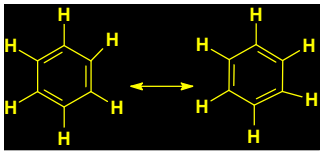


Aromatic Compounds and Benzene

Aromatic compounds contain benzene.

Benzene, C_6H_6, is represented as a six carbon ring with 3 double bonds.

Two possible can be drawn to show benzene in this form.



Naming Aromatic Compounds

Aromatic compounds are named with *benzene as the parent chain*. One side group is named in front of the name *benzene*.

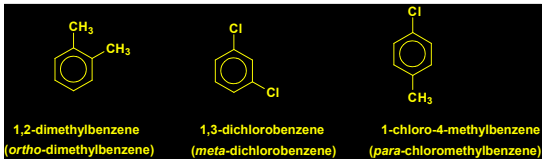
- No number is needed for mono-substituted benzene since all the ring positions are identical.

methylbenzene (toluene)

chlorobenzene

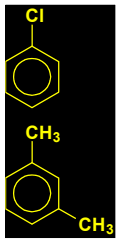
Naming Aromatic Compounds

When two groups are attached to benzene, the ring is numbered to give the lower numbers to the side groups. The prefixes *ortho (1,2), meta (1,3-)* and *para (1,4-)* are also used.



Learning Check

Select the names for each structure:

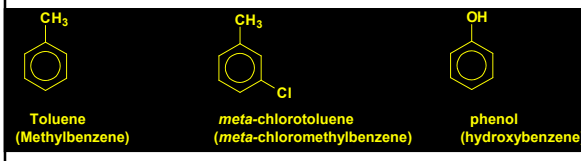


a. Chlorocyclohexane
b. Chlorobenzene
c. 1-chlorobenzene

a. *Meta*-xylene
b. *Meta*-dimethylbenzene
c. 1,3-dimethylbenzene

Some Common Names

Some substituted benzene rings also use a common name. Then naming with additional more side groups uses the *ortho-, meta-, para-* system.



Learning Check

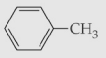
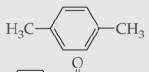
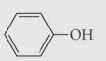
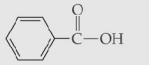
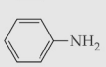
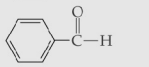
Write the structural formulas for each of the following:

A. 1,3-dichlorobenzene

B. *Ortho*-chlorotoluene

- Many substituted aromatic compounds have common names in addition to their systematic names.

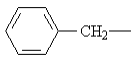
TABLE 13.2 Common Names of Some Aromatic Compounds

Structure	Name	Structure	Name
	Toluene		*para*-Xylene
	Phenol		Benzoic acid
	Aniline		Benzaldehyde

New Attached Groups

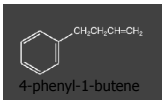
- Phenyl

- Benzyl

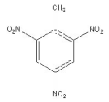


- Nitro -NO_2

Refer to your chart for order of priority!



4-phenyl-1-butene


2,4,6-trinitrotoluene